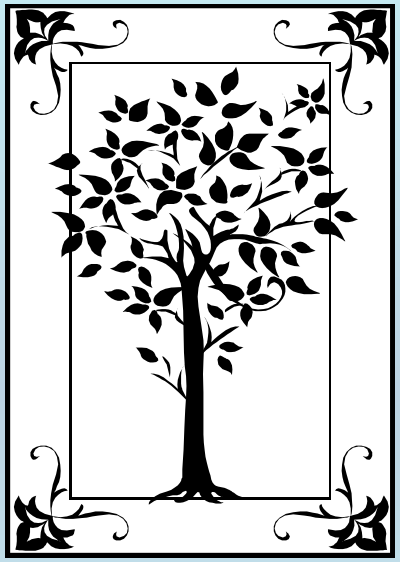
METADATA AND NUMERICAL DATA CAPTURE:
Excess Volume: $V^E_{m,12}$
(2 – Components)

Guided Data Capture (GDC)



This tutorial describes
METADATA AND NUMERICAL DATA CAPTURE:
for **2-component**
EXCESS VOLUME: $V^E_{m,12}$
with the Guided Data Capture (GDC) software.

NOTE:

The tutorials proceed sequentially to ease the descriptions. It is not necessary to enter *all* compounds before entering *all* samples, etc.

Compounds, samples, properties, etc., can be added or modified at any time.

However, the hierarchy must be maintained (i.e., a property cannot be entered, if there is no associated sample or compound.)

The experimental data used in this example is from:

128 *J. Chem. Eng. Data* 1997, *42*, 128−131

Binary Mixtures of Butanol + Pentane, + Hexane, + Heptane, + Octane, + 2,2,4-Trimethylpentane, and + Carbon Tetrachloride. 1. Excess Molar Volumes at 288.15 K and 298.15 K and Refractive Indexes at 298.15 K

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Excess molar volumes, V_m^E, have been measured for binary mixtures of butanol (n-C_4H_9OH) + pentane (n-C_5H_{12}), + hexane (n-C_6H_{14}), + heptane (n-C_7H_{16}), + octane (n-C_8H_{18}), + 2,2,4-trimethylpentane (2,2,4-TMP), and + carbon tetrachloride (CCl_4) at 288.15 K and 298.15 K, and refractive indexes, n_D, have been measured for these mixtures at 298.15 K. At both temperatures V_m^E has been found to be positive throughout the entire range of composition for $x$$n$-$C_4H_9OH$ + $(1 - x)$$n$-$C_7H_{16}$ and + $(1 - x)$$n$-$C_8H_{18}$. At both temperatures 288.15 K and 298.15 K, V_m^E is positive at low mole fractions of n-C_4H_9OH and negative at its higher mole fractions in the case of mixtures of n-C_4H_9OH with n-C_5H_{12}, n-C_6H_{14}, 2,2,4-TMP, and CCl_4. Values of V_m^E and n_D for the various mixtures of n-C_4H_9OH have been fitted in smoothing equations.

Excess Volume ($V^E_{m,12}$) for the binary system
1-butanol + n-pentane
at p = 101.3 kPa and T = 288.15 K and 298.15 K

Table 1. Experimental Values of the Excess Molar Volumes, V_m^E, for n-C_4H_9OH + n-C_5H_{12}, + n-C_6H_{14}, + n-C_7H_{16}, + n-C_8H_{18}, + 2,2,4-TMP, and + CCl_4 at 288.15 and 298.15 K

x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}
			$x$$n$-$C_4H_9OH$ + (1 − x)n-C_5H_{12}				
			T = 288.15 K				
0.0442	0.025	0.3024	−0.096	0.5398	−0.276	0.7976	−0.192
0.0709	0.037	0.3232	−0.117	0.5823	−0.284	0.8466	−0.144
0.1186	0.036	0.3727	−0.160	0.6240	−0.282	0.9392	−0.048
0.1733	0.017	0.4118	−0.198	0.7055	−0.259		
0.2811	−0.071	0.5141	−0.261	0.7536	−0.228		
			T = 298.15 K				
0.0440	0.031	0.2769	−0.073	0.5696	−0.245	0.8914	−0.119
0.0700	0.039	0.3341	−0.116	0.6539	−0.251	0.9388	−0.069
0.1193	0.030	0.3960	−0.167	0.7108	−0.243		
0.2046	−0.020	0.4780	−0.209	0.7652	−0.219		
0.2302	−0.037	0.5180	−0.229	0.8404	−0.168		

This data set is considered here.

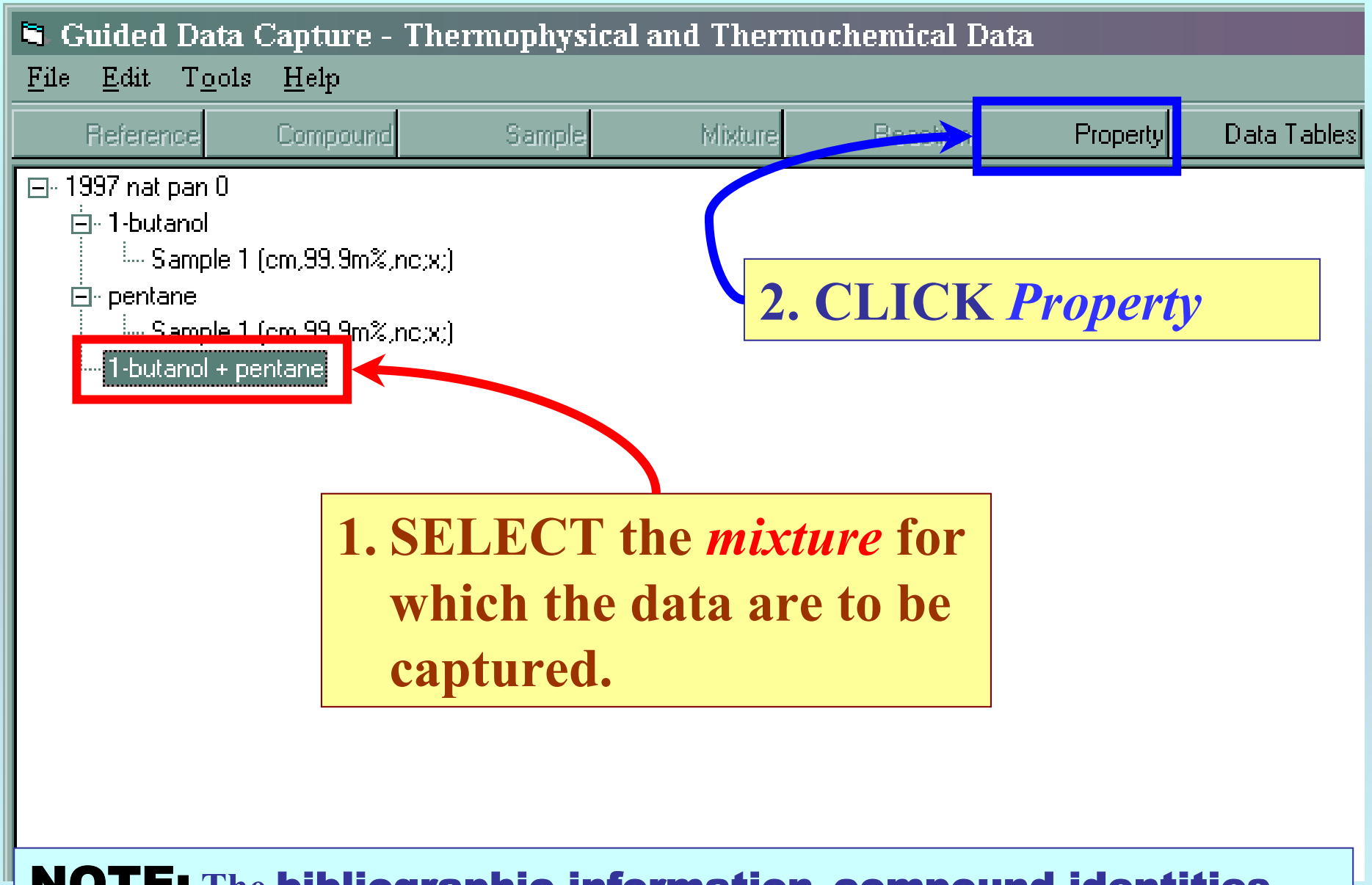
NOTE: This data could be captured as two data sets with temperature constrained in each, but here temperature will be included as a variable. Generally, operation of the GDC software is easier (*i.e.*, less repetitious), if the number of separate data sets is minimized.

Experimental Method Info:

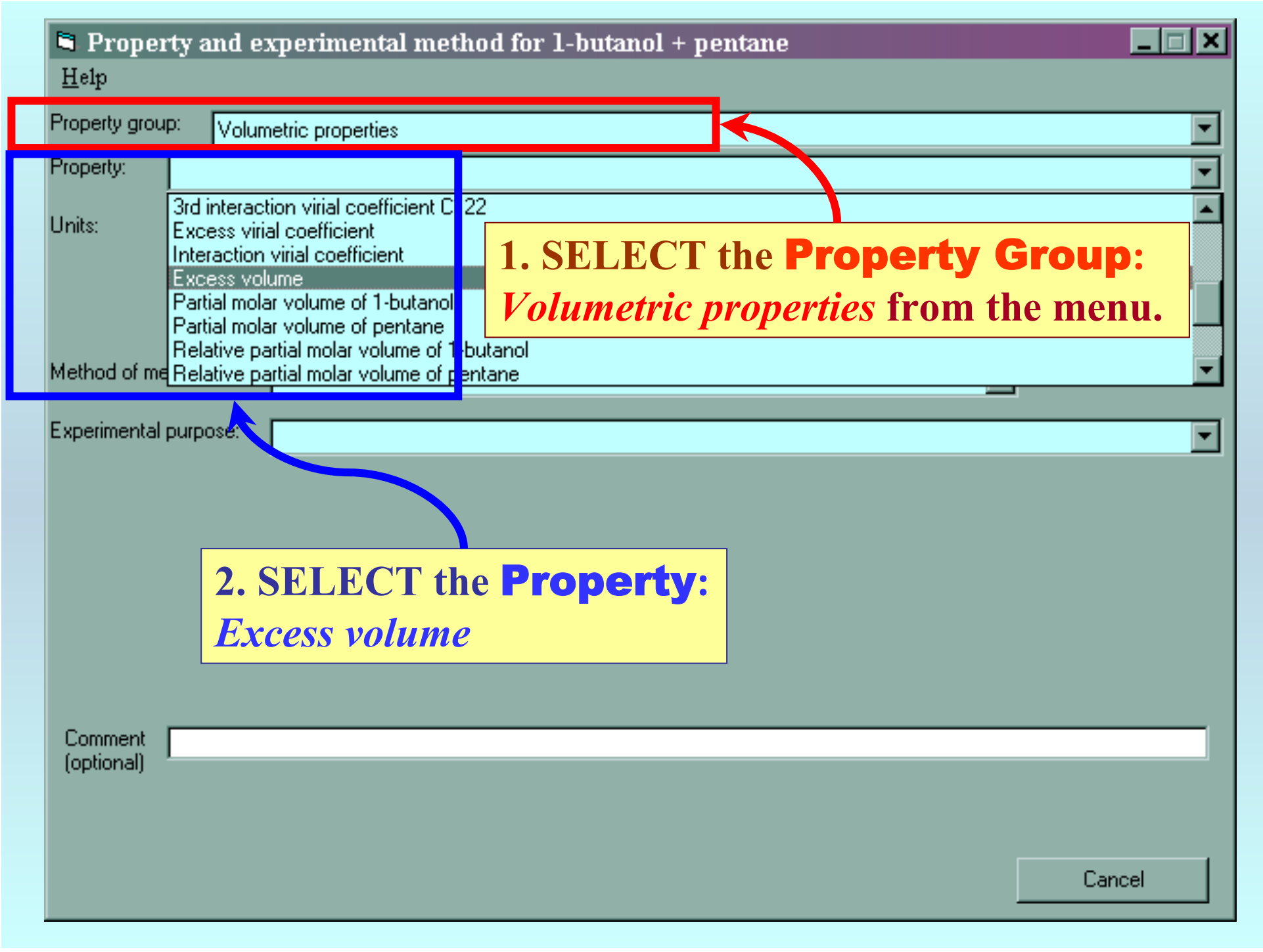
Methods. (i) Excess molar volumes, V_m^E, were measured with an imprecision of the order of ± 0.002 $cm^3 \cdot mol^{-1}$ using a two-limbed Pyrex glass dilatometer which was similar to that used in earlier measurements (Nath and Chaudhary, 1992; Nath and Rashmi, 1990).

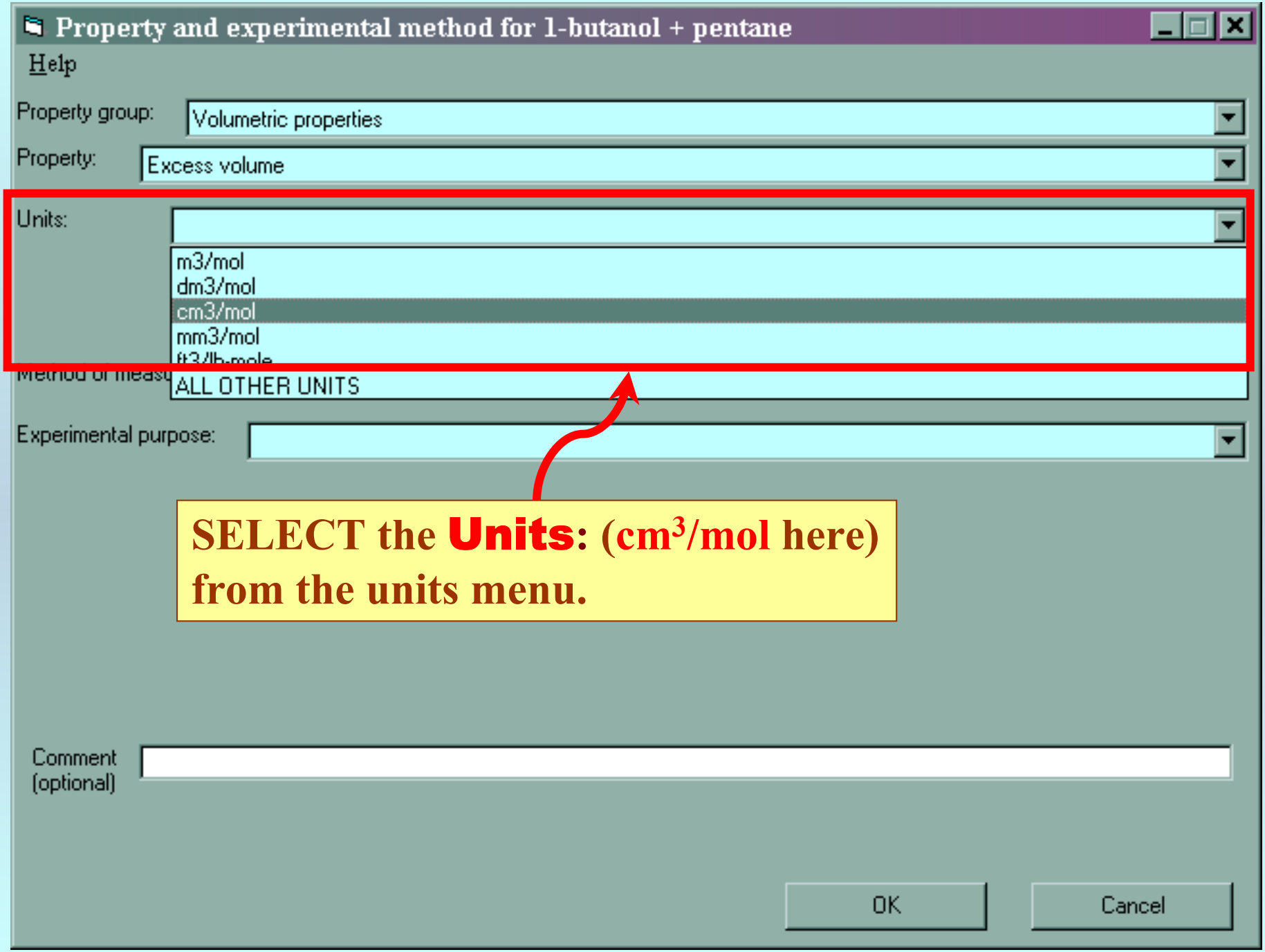
The dilatometer (mounted on a stand) was immersed in a thermostat which was controlled to ± 0.01 K.

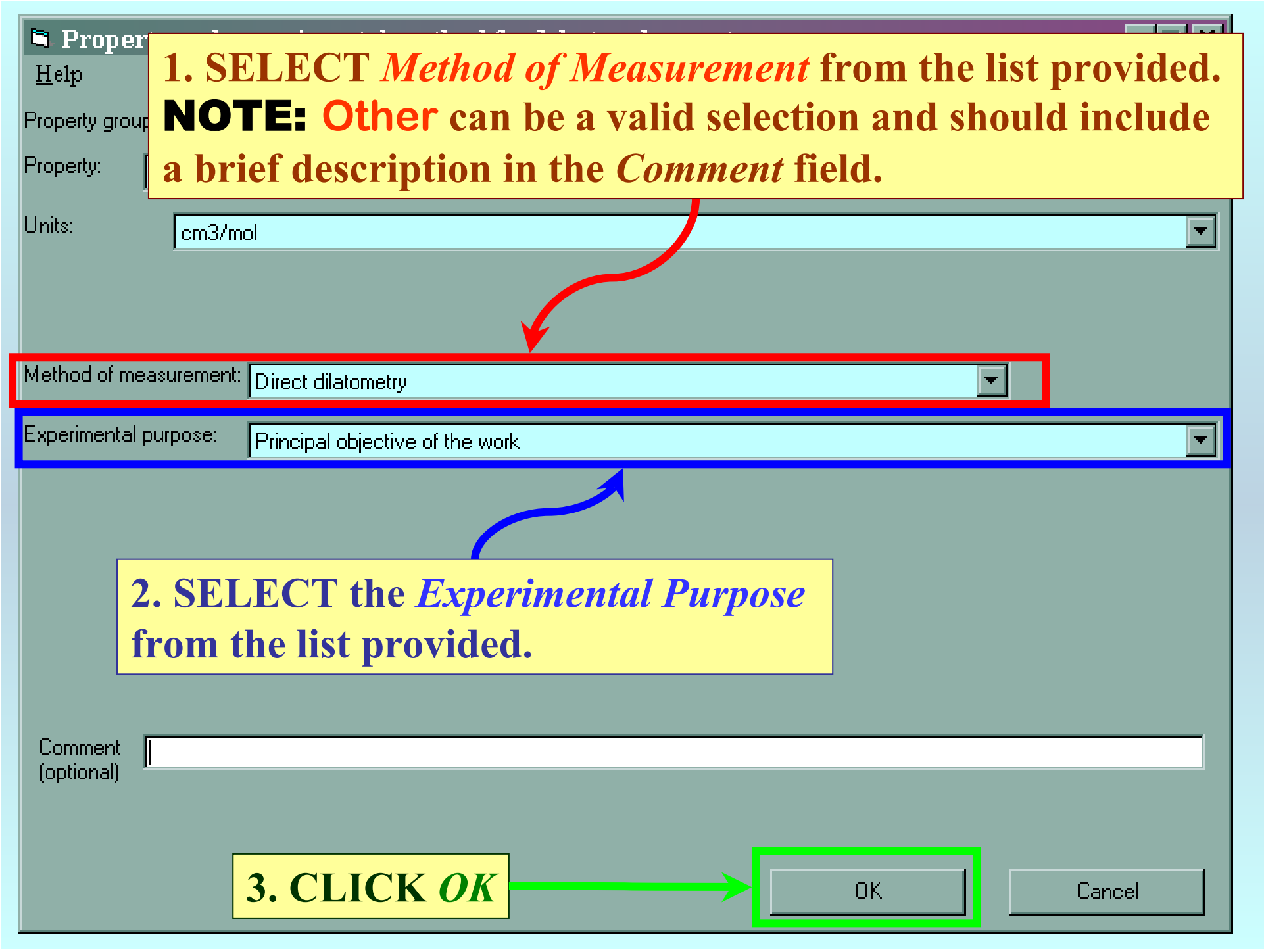
Uncertainty estimate:



NOTE: The **bibliographic information**, **compound identities**, **sample descriptions**, and **mixture** were entered previously. (There are separate tutorials, which describe capture of this information, if needed.)


Property and experimental method for 1-butanol + pentane
Help
Property group:
Volumetric properties
Property:
Units:
3rd interaction virial coefficient C 22
Excess virial coefficient
Interaction virial coefficient
Excess volume
Partial molar volume of 1-butanol
Partial molar volume of pentane
Relative partial molar volume of 1-butanol
Relative partial molar volume of pentane
Method of me
Experimental purpose:
1. SELECT the Property Group:
Volumetric properties from the menu.
2. SELECT the Property:
Excess volume
Comment
(optional)
Cancel


Property and experimental method for 1-butanol + pentane
Help
Property group:
Volumetric properties
Property:
Excess volume
Units:
m3/mol
dm3/mol
cm3/mol
mm3/mol
ALL OTHER UNITS
Experimental purpose:
SELECT the Units: (cm3/mol here) from the units menu.
Comment (optional)
OK
Cancel

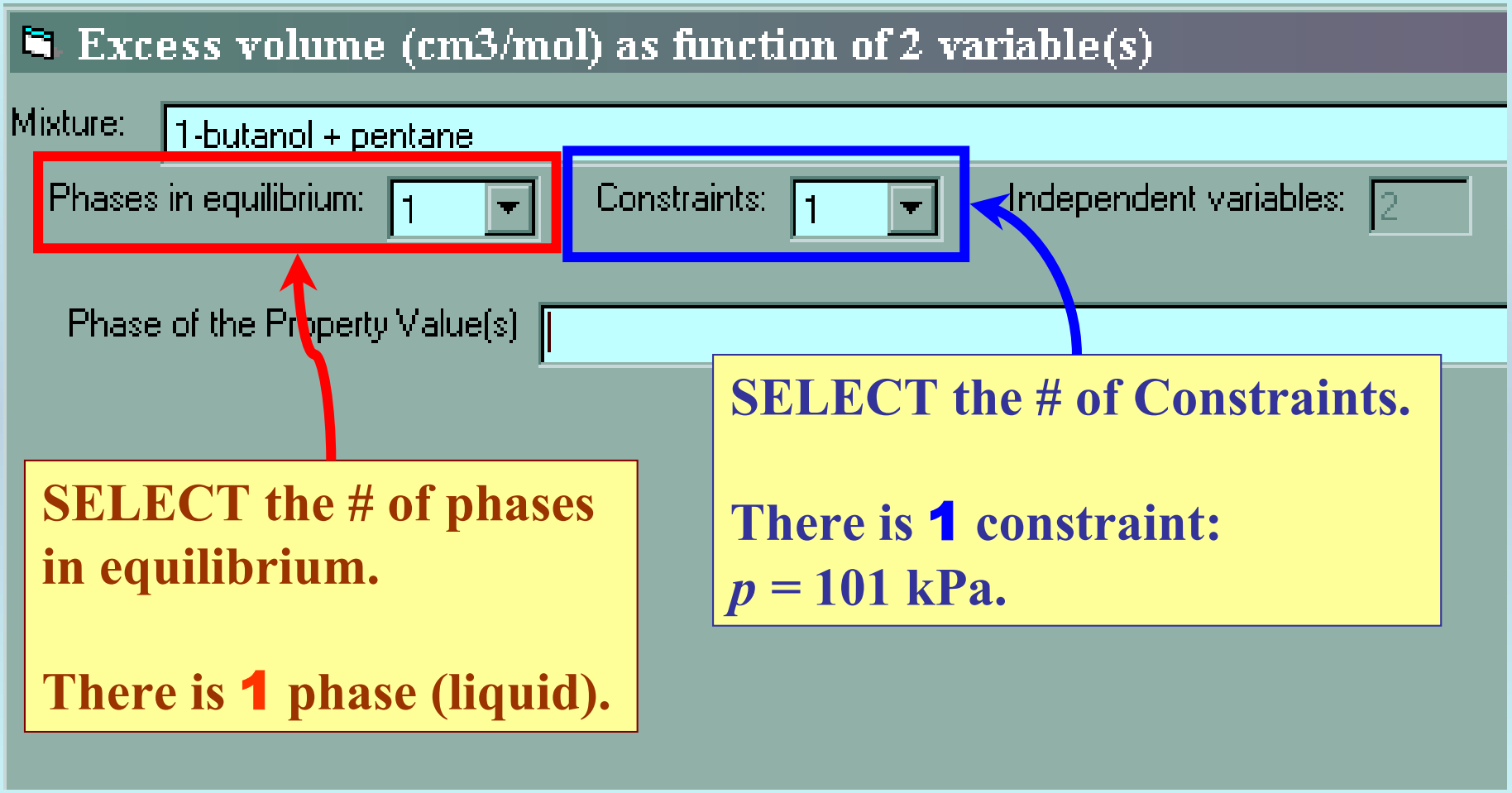


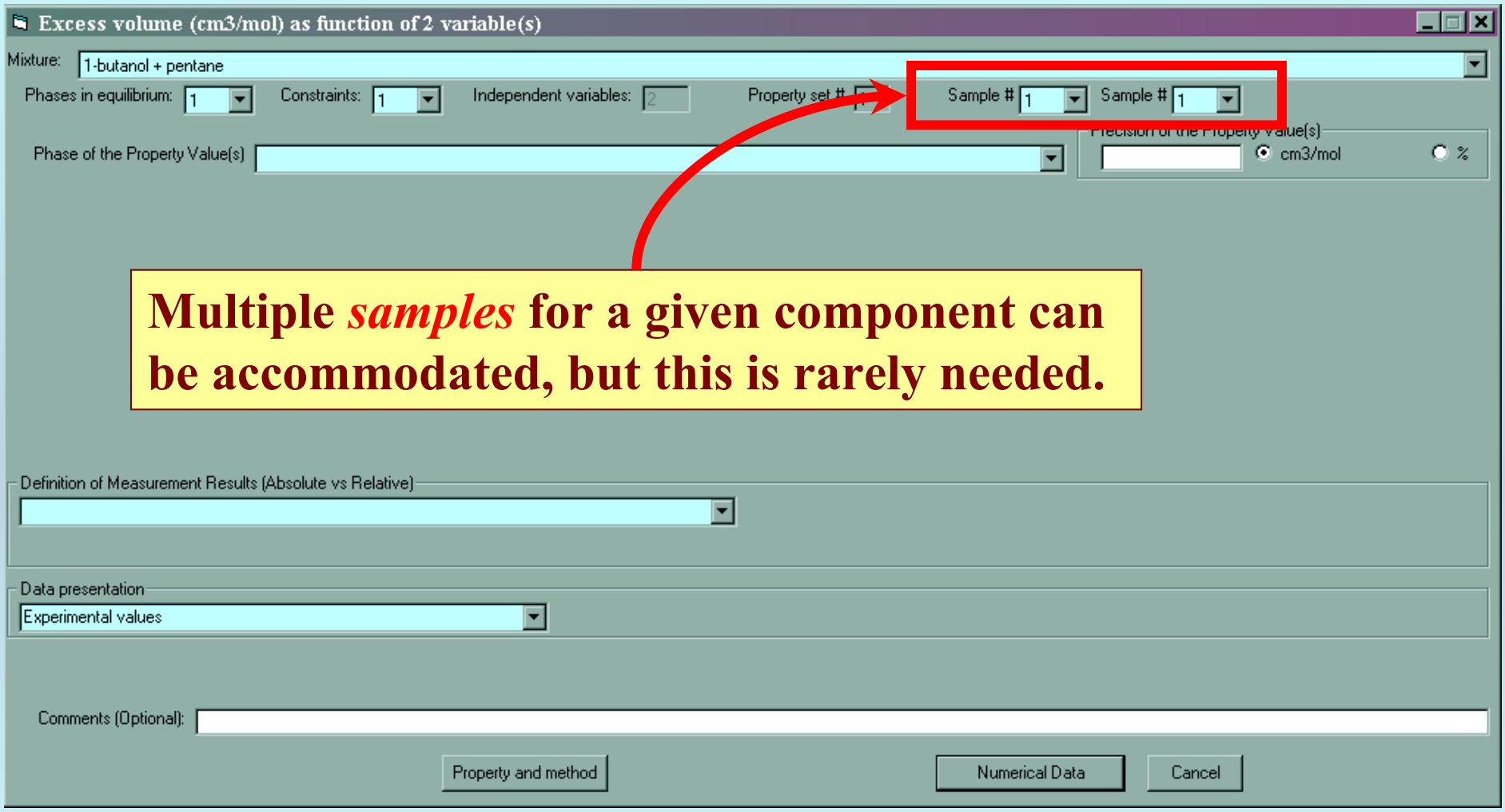
1. SELECT *Method of Measurement* from the list provided.
NOTE: Other can be a valid selection and should include a brief description in the *Comment* field.

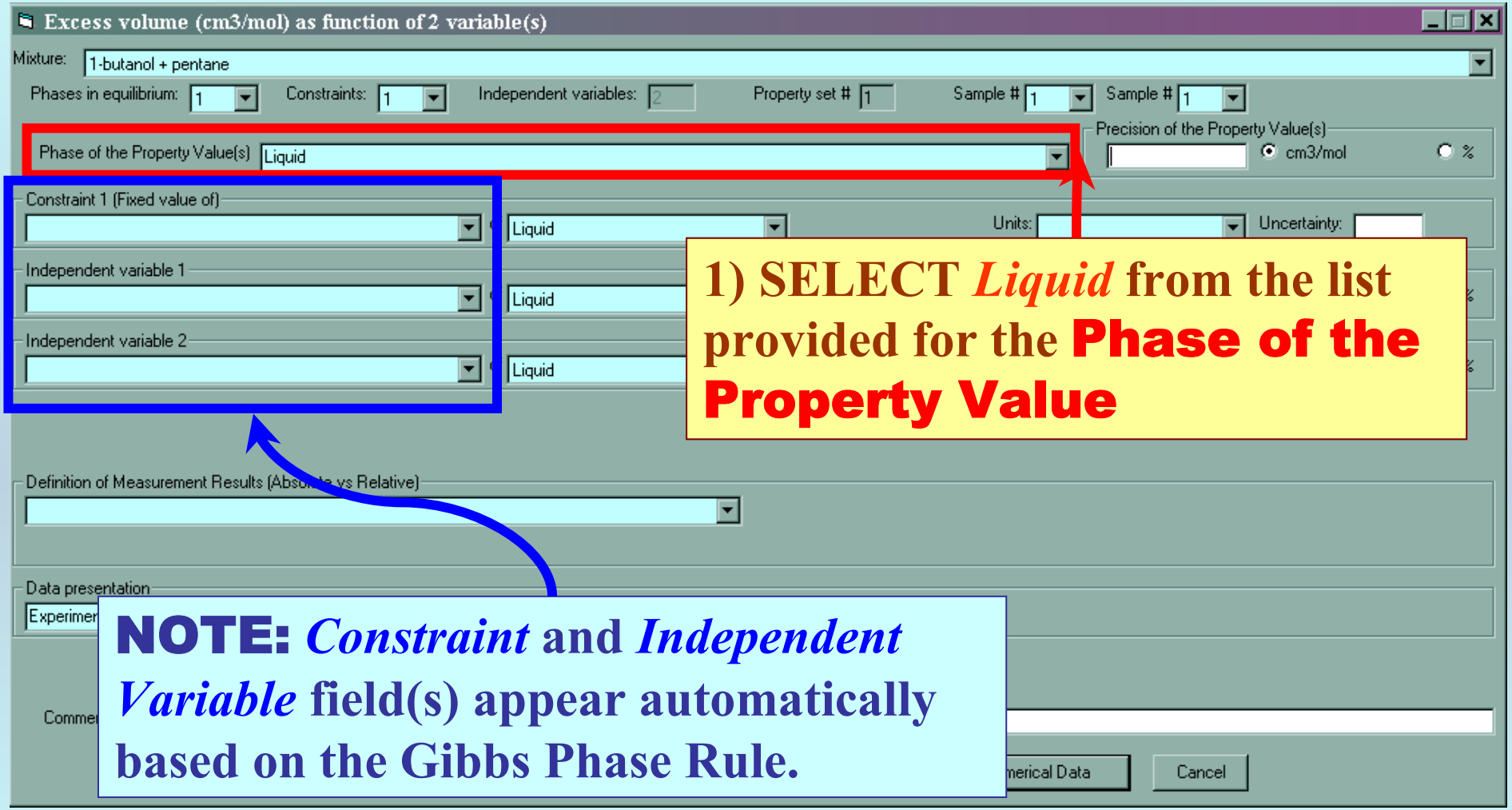
2. SELECT the *Experimental Purpose* from the list provided.

3. CLICK *OK*

SELECTION of # of Phases in Equilibrium and # of Constraints

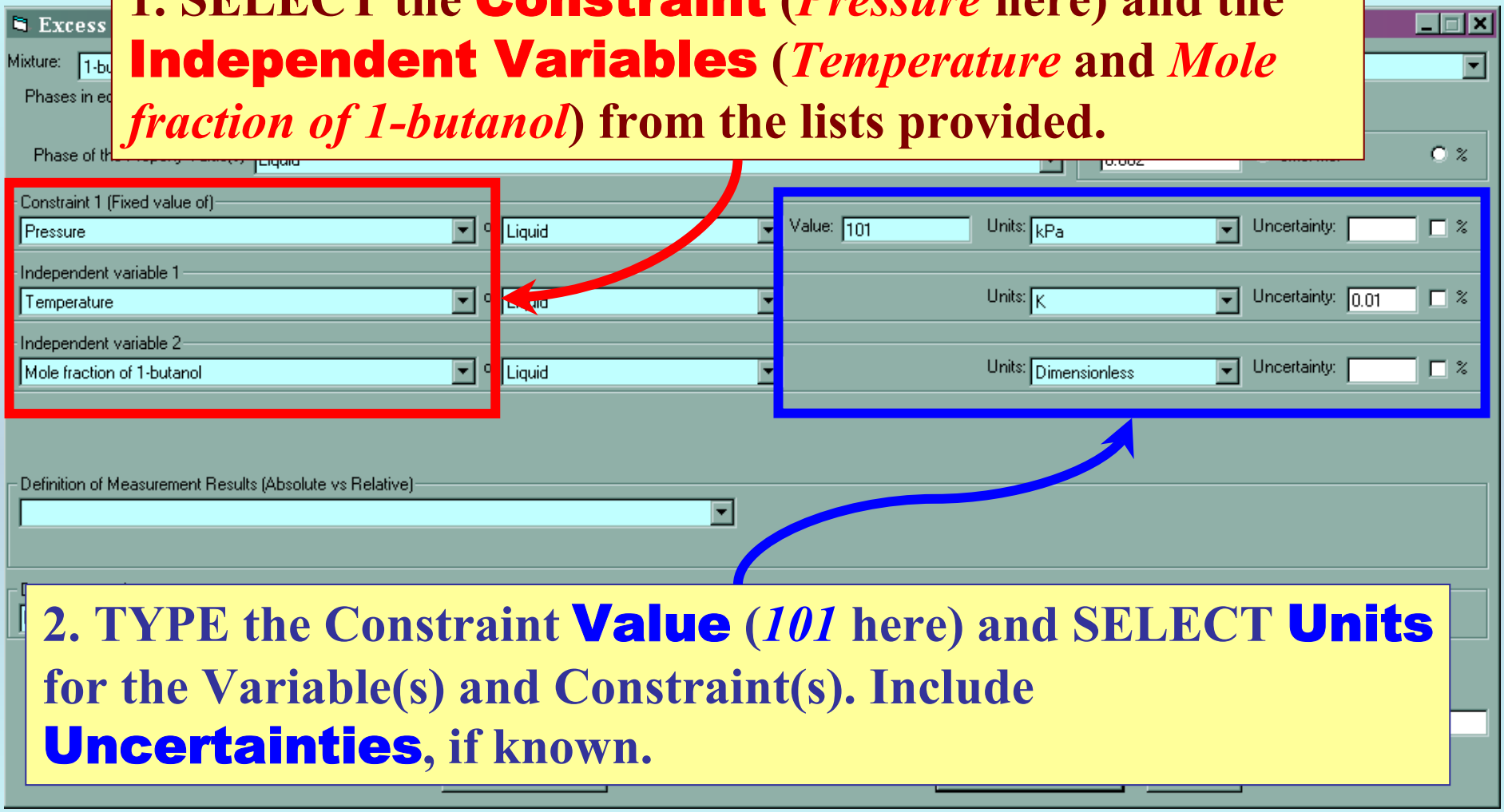



Excess volume (cm3/mol) as function of 2 variable(s)
Mixture:
1-butanol + pentane
Phases in equilibrium:
1
Constraints:
1
Independent variables:
2
Property set #
Sample #
1
Sample #
1
Phase of the Property Value(s)
Precision of the Property Value(s)
cm3/mol
%
Multiple samples for a given component can be accommodated, but this is rarely needed.
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimental values
Comments (Optional):
Property and method
Numerical Data
Cancel


Excess volume (cm3/mol) as function of 2 variable(s)
Mixture:
1-butanol + pentane
Phases in equilibrium:
Constraints:
Independent variables:
Property set #
Sample #
Sample #
Phase of the Property Value(s)
Liquid
Precision of the Property Value(s)
cm3/mol
%
Constraint 1 (Fixed value of)
Liquid
Units:
Uncertainty:
Independent variable 1
Liquid
Independent variable 2
Liquid
Definition of Measurement Results (Absolute vs Relative)
Data presentation
Experimer
Comme
merical Data
Cancel
1) SELECT Liquid from the list provided for the Phase of the Property Value
NOTE: Constraint and Independent Variable field(s) appear automatically based on the Gibbs Phase Rule.

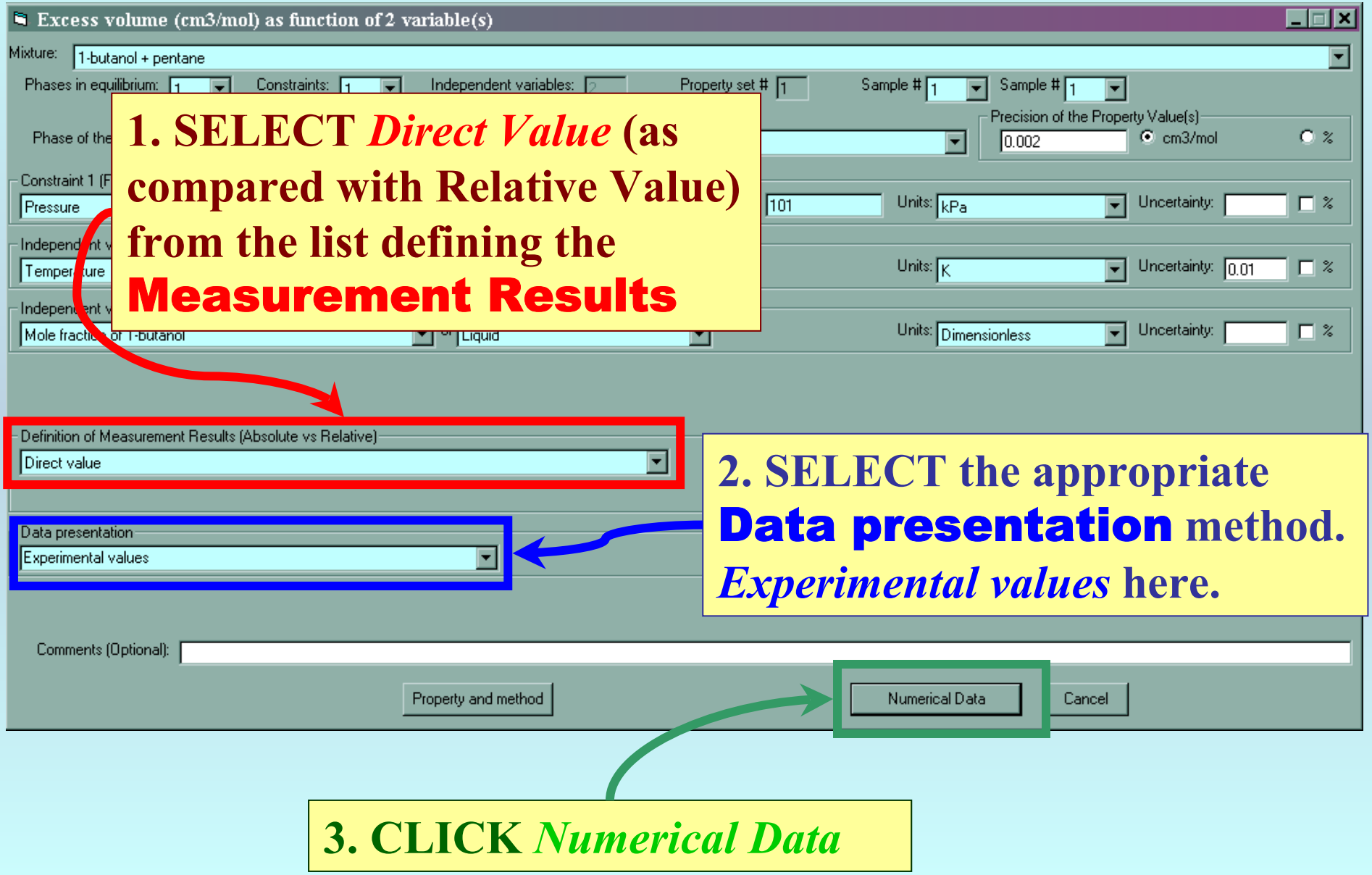
Specification of constraints, constraint values, and constraint units

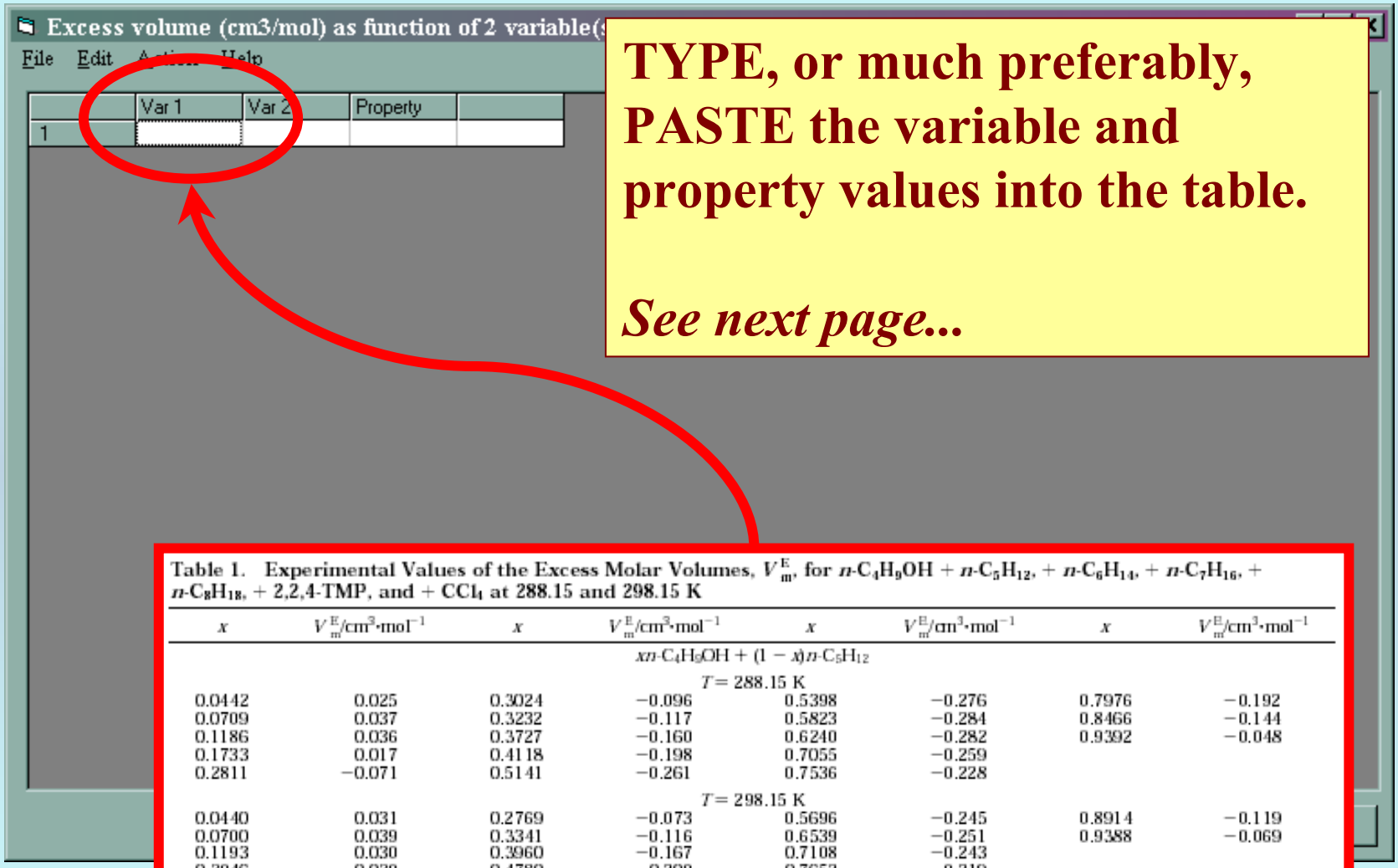
1. SELECT the **Constraint** (*Pressure* here) and the **Independent Variables** (*Temperature* and *Mole fraction of 1-butanol*) from the lists provided.



2. TYPE the Constraint **Value** (*101* here) and SELECT **Units** for the Variable(s) and Constraint(s). Include **Uncertainties**, if known.

Measurement definition and Data presentation





TYPE, or much preferably, PASTE the variable and property values into the table.

See next page...

Table 1. Experimental Values of the Excess Molar Volumes, V_m^E, for n-C_4H_9OH + n-C_5H_{12}, + n-C_6H_{14}, + n-C_7H_{16}, + n-C_8H_{18}, + 2,2,4-TMP, and + CCl_4 at 288.15 and 298.15 K

x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}
			$x$$n$-$C_4H_9OH$ + (1 − x)n-C_5H_{12}				
			T = 288.15 K				
0.0442	0.025	0.3024	−0.096	0.5398	−0.276	0.7976	−0.192
0.0709	0.037	0.3232	−0.117	0.5823	−0.284	0.8466	−0.144
0.1186	0.036	0.3727	−0.160	0.6240	−0.282	0.9392	−0.048
0.1733	0.017	0.4118	−0.198	0.7055	−0.259		
0.2811	−0.071	0.5141	−0.261	0.7536	−0.228		
			T = 298.15 K				
0.0440	0.031	0.2769	−0.073	0.5696	−0.245	0.8914	−0.119
0.0700	0.039	0.3341	−0.116	0.6539	−0.251	0.9388	−0.069
0.1193	0.030	0.3960	−0.167	0.7108	−0.243		
0.2046	−0.020	0.4780	−0.209	0.7652	−0.219		
0.2302	−0.037	0.5180	−0.229	0.8404	−0.168		

Excess volume (cm3/mol) as function of 2 variable(s)

File Edit Action Help

	Var 1	Var 2	Property
1	288.15	0.0442	0.025
2	288.15	0.0709	0.037
3	288.15	0.1186	0.036
4	288.15	0.1733	0.017
5	288.15	0.2811	-0.071
6	288.15	0.3024	-0.096
7	288.15	0.3232	-0.117
8	288.15	0.3727	-0.160
9	288.15	0.4118	-0.198
10	288.15	0.5141	-0.261
11	288.15	0.5398	-0.276
12	288.15	0.5823	-0.284
13	288.15	0.6240	-0.282
14	288.15	0.7055	-0.259
15	288.15	0.7536	-0.228
16	288.15	0.7	
17	288.15	0.8	
18	288.15	0.9	
19	298.15	0.0	
20	298.15	0.0	
21	298.15	0.1	
22	298.15	0.2	
23	298.15	0.2	
24	298.15	0.2	
25	298.15	0.3	

Table 1. Experimental Values of t… olar Volumes, V_m^E, for n-C_4H_9OH + n-C_5H_{12}, + n-C_6H_{14}, + n-C_7H_{16}, + n-C_8H_{18}, + 2,2,4-TMP, and + CCl_4 at 28… 8.15 K

x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}	x	V_m^E/cm^3·mol^{-1}
			xn-C_4H_9OH + $(1-x)n$-C_5H_{12}				
			T = 288.15 K				
0.0442	0.025	0.3024	−0.096	0.5398	−0.276	0.7976	−0.192
0.0709	0.037	0.3232	−0.117	0.5823	−0.284	0.8466	−0.144
0.1186	0.036	0.3727	−0.160	0.6240	−0.282	0.9392	−0.048
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0.2811	−0.071	0.5141	−0.261	0.7536	−0.228		
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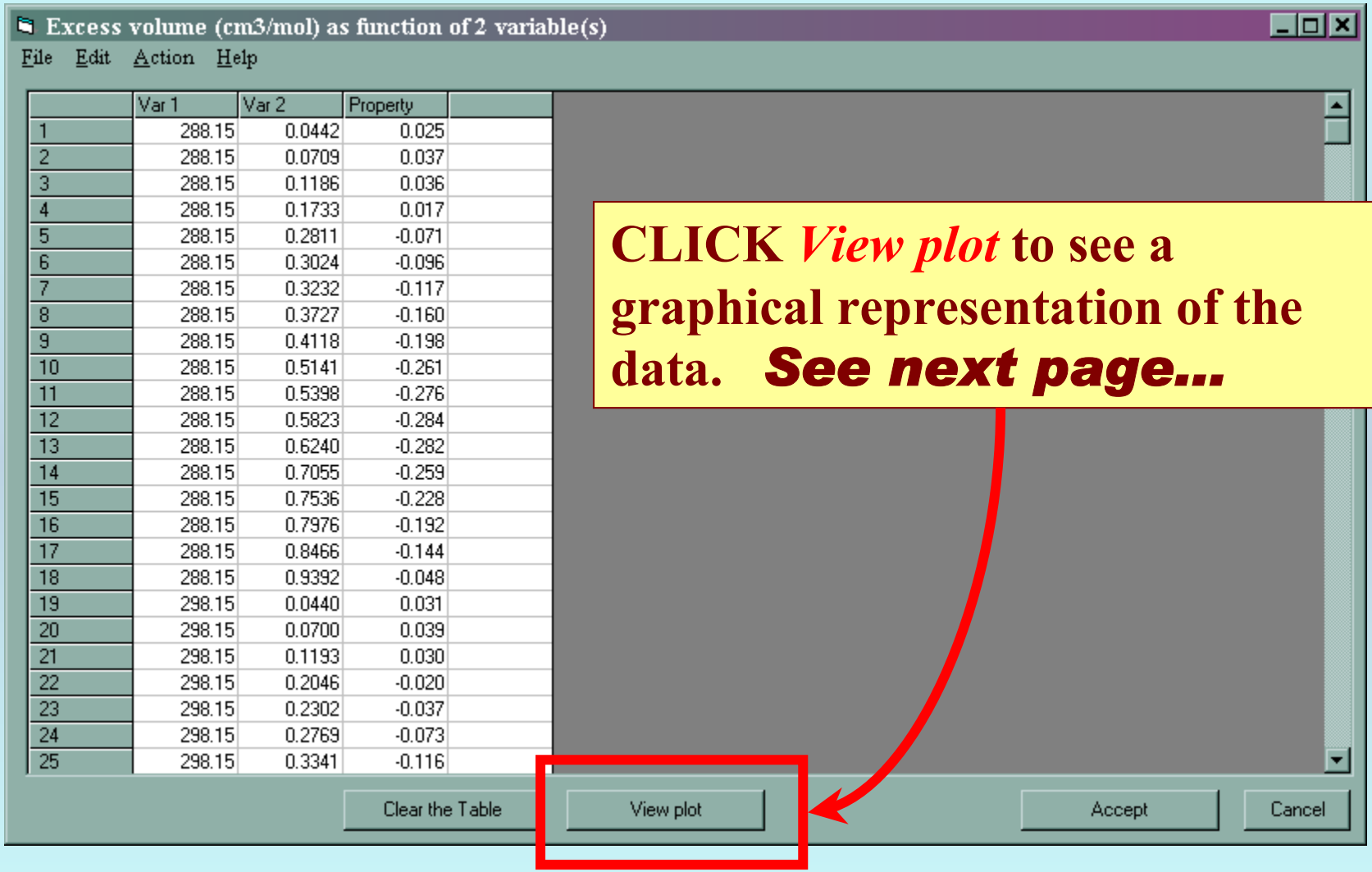
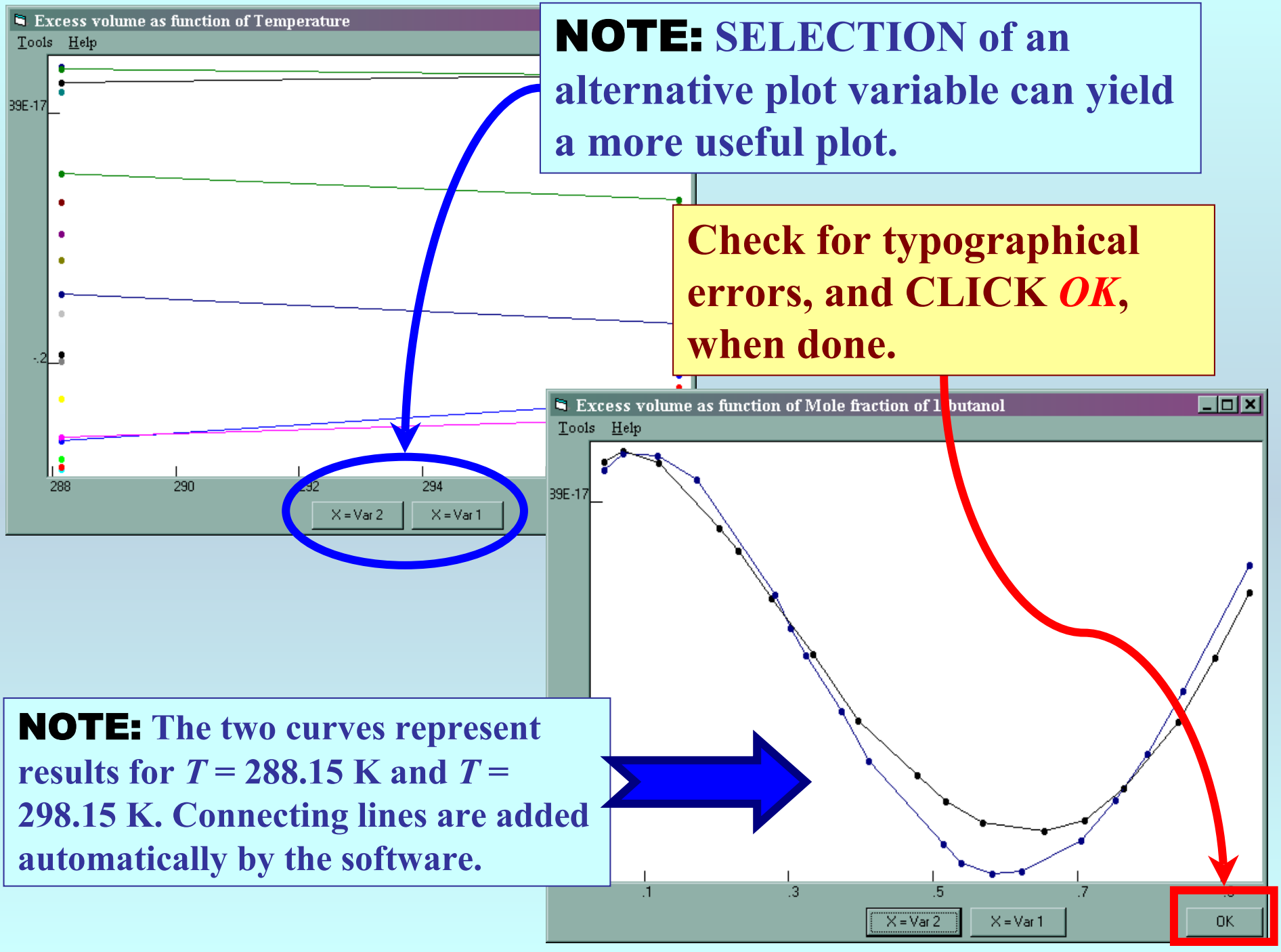
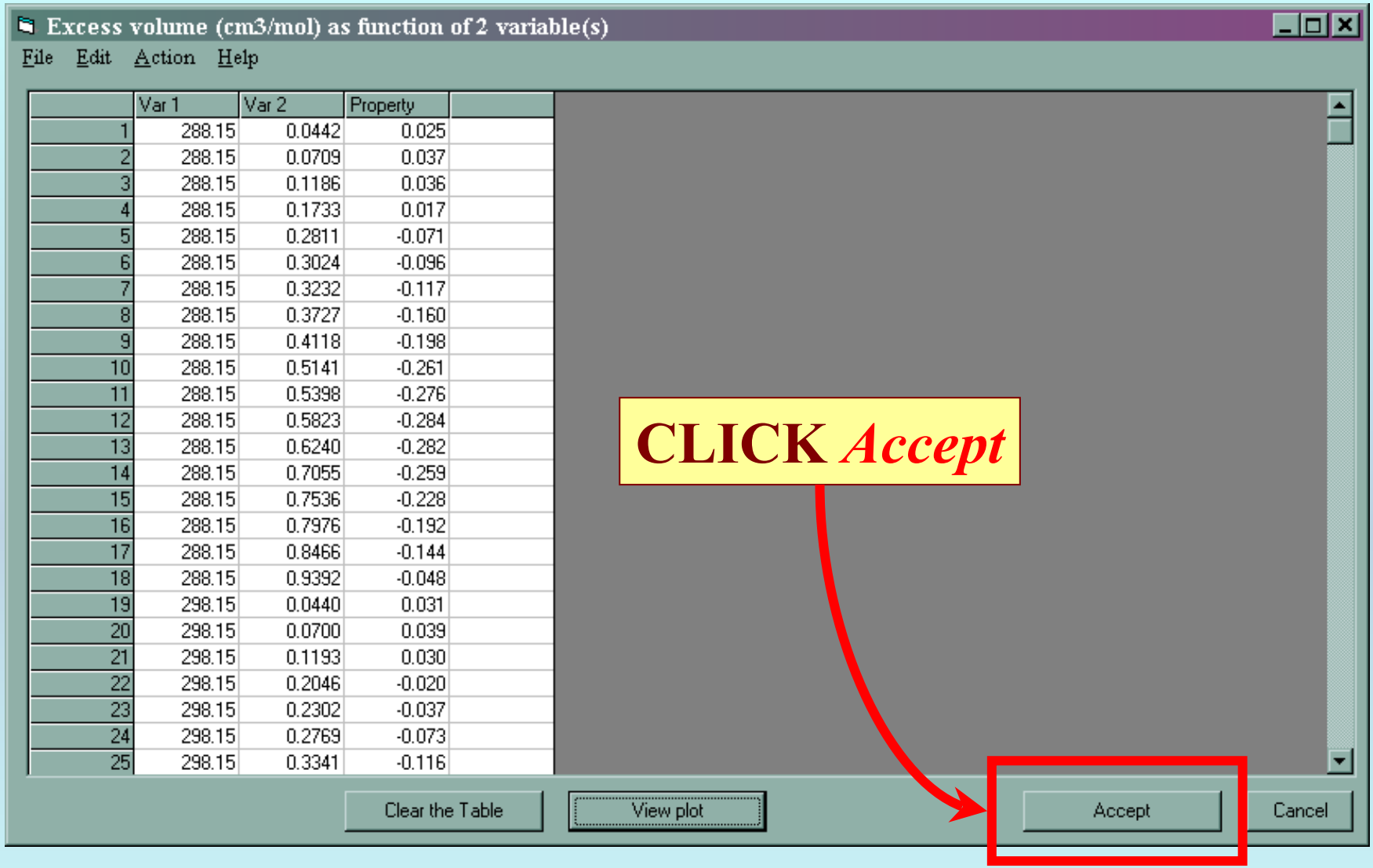
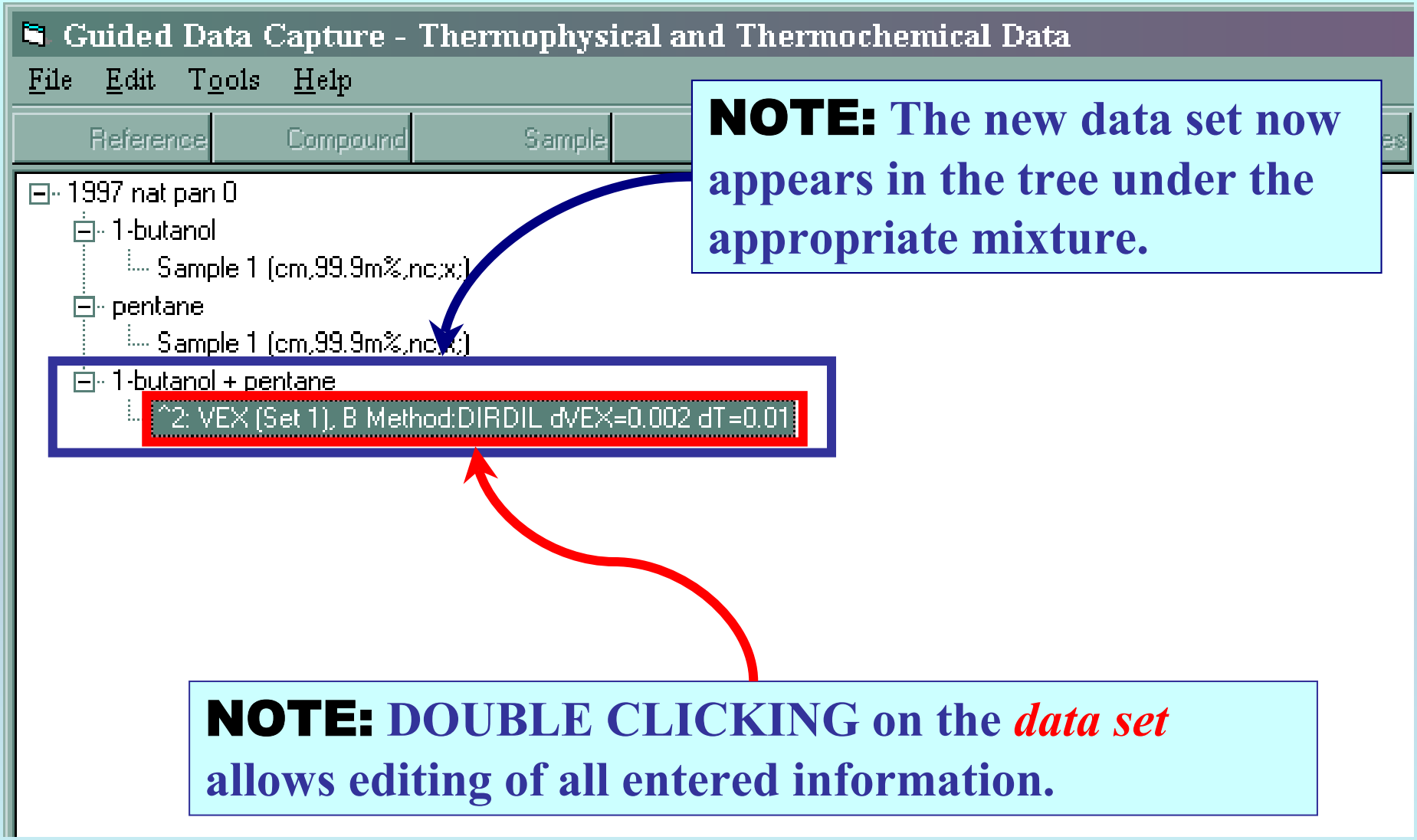
0.0700	0.039	0.3341	−0.116	0.6539	−0.251	0.9388	−0.069
0.1193	0.030	0.3960	−0.167	0.7108	−0.243		
0.2046	−0.020	0.4780	−0.209	0.7652	−0.219		
0.2302	−0.037	0.5180	−0.229	0.8404	−0.168		

NOTE: Simple CUT/PASTE procedures can be used within the table to convert the original table into the required number of columns. (This can also be done externally in spreadsheet software, e.g., EXCEL.)


Excess volume (cm3/mol) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 288.15 0.0442 0.025
2 288.15 0.0709 0.037
3 288.15 0.1186 0.036
4 288.15 0.1733 0.017
5 288.15 0.2811 -0.071
6 288.15 0.3024 -0.096
7 288.15 0.3232 -0.117
8 288.15 0.3727 -0.160
9 288.15 0.4118 -0.198
10 288.15 0.5141 -0.261
11 288.15 0.5398 -0.276
12 288.15 0.5823 -0.284
13 288.15 0.6240 -0.282
14 288.15 0.7055 -0.259
15 288.15 0.7536 -0.228
16 288.15 0.7976 -0.192
17 288.15 0.8466 -0.144
18 288.15 0.9392 -0.048
19 298.15 0.0440 0.031
20 298.15 0.0700 0.039
21 298.15 0.1193 0.030
22 298.15 0.2046 -0.020
23 298.15 0.2302 -0.037
24 298.15 0.2769 -0.073
25 298.15 0.3341 -0.116
CLICK View plot to see a graphical representation of the data. See next page...
Clear the Table
View plot
Accept
Cancel


Excess volume as function of Temperature
Tools Help
39E-17
-.2
288
290
292
294
X = Var 2
X = Var 1
NOTE: SELECTION of an alternative plot variable can yield a more useful plot.
Check for typographical errors, and CLICK OK, when done.
Excess volume as function of Mole fraction of 1 butanol
Tools Help
39E-17
.1
.3
.5
.7
X = Var 2
X = Var 1
OK
NOTE: The two curves represent results for T = 288.15 K and T = 298.15 K. Connecting lines are added automatically by the software.


Excess volume (cm3/mol) as function of 2 variable(s)
File Edit Action Help
Var 1 Var 2 Property
1 288.15 0.0442 0.025
2 288.15 0.0709 0.037
3 288.15 0.1186 0.036
4 288.15 0.1733 0.017
5 288.15 0.2811 -0.071
6 288.15 0.3024 -0.096
7 288.15 0.3232 -0.117
8 288.15 0.3727 -0.160
9 288.15 0.4118 -0.198
10 288.15 0.5141 -0.261
11 288.15 0.5398 -0.276
12 288.15 0.5823 -0.284
13 288.15 0.6240 -0.282
14 288.15 0.7055 -0.259
15 288.15 0.7536 -0.228
16 288.15 0.7976 -0.192
17 288.15 0.8466 -0.144
18 288.15 0.9392 -0.048
19 298.15 0.0440 0.031
20 298.15 0.0700 0.039
21 298.15 0.1193 0.030
22 298.15 0.2046 -0.020
23 298.15 0.2302 -0.037
24 298.15 0.2769 -0.073
25 298.15 0.3341 -0.116
CLICK Accept
Clear the Table
View plot
Accept
Cancel


Guided Data Capture - Thermophysical and Thermochemical Data
File Edit Tools Help
Reference Compound Sample
1997 nat pan 0
1-butanol
Sample 1 (cm,99.9m%,nc;x;)
pentane
Sample 1 (cm,99.9m%,nc;x;)
1-butanol + pentane
^2: VEX (Set 1), B Method:DIRDIL dVEX=0.002 dT=0.01
NOTE: The new data set now appears in the tree under the appropriate mixture.
NOTE: DOUBLE CLICKING on the data set allows editing of all entered information.

END

Continue with other compounds, samples, properties, reactions, etc...

***or* save your file and exit the program.**